

## LA-UR-19-21889

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Title: Nonequilibrium Transport in Nonlinear Media: Collective and Diffusive  
Thermal Transport in DNA

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Intended for: Report

Issued: 2019-03-04

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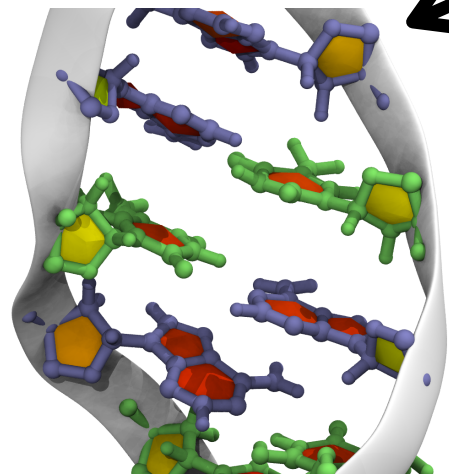
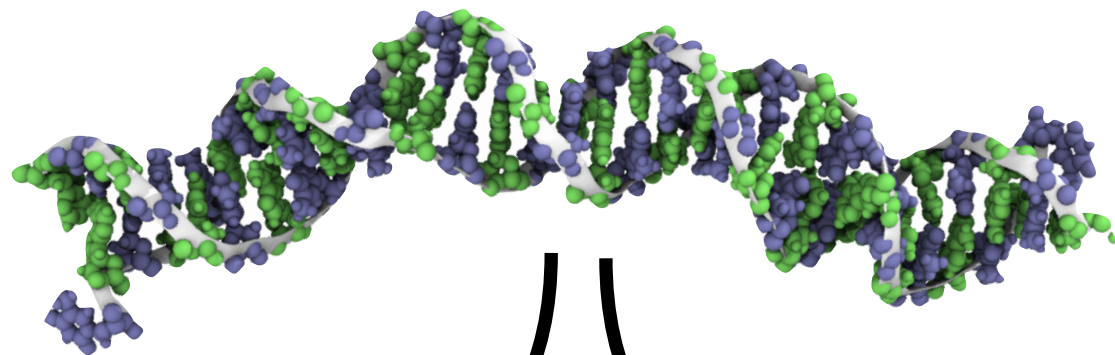
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# Nonequilibrium Transport in Nonlinear Media:

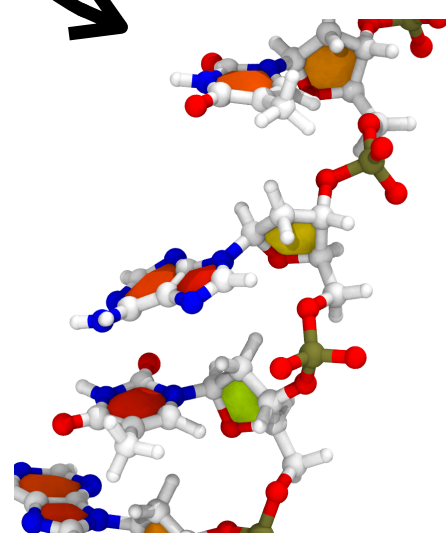
PI: K. A. Velizhanin

## Collective and Diffusive Thermal Transport in DNA

Vibrational transport in DNA is mediated by an interplay between multiple nonlinear pathways

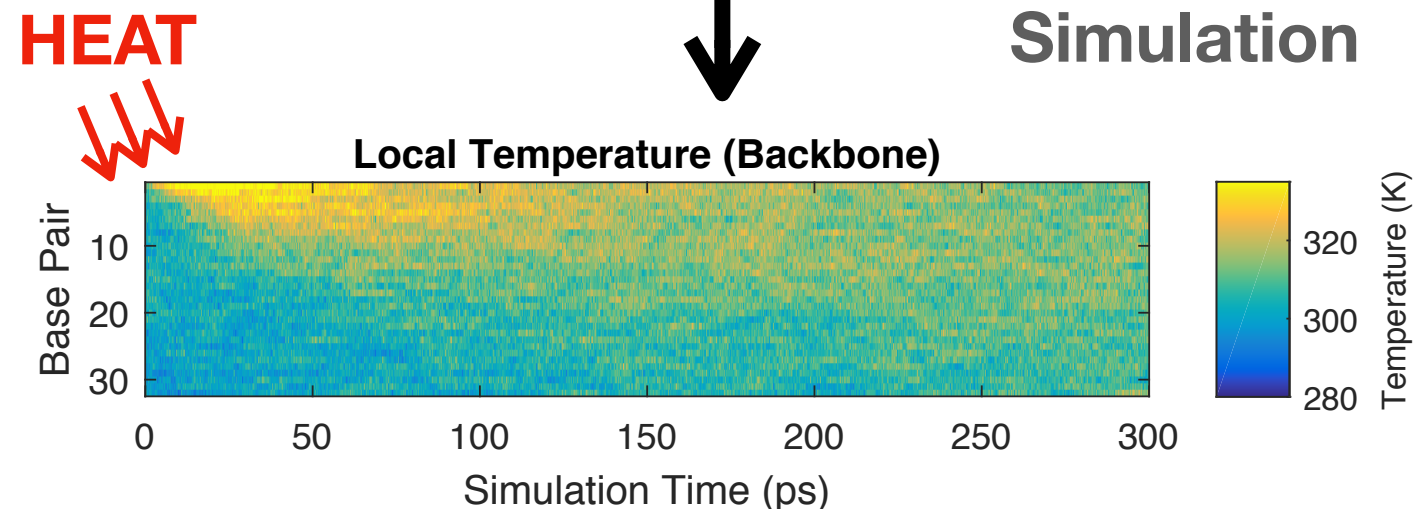
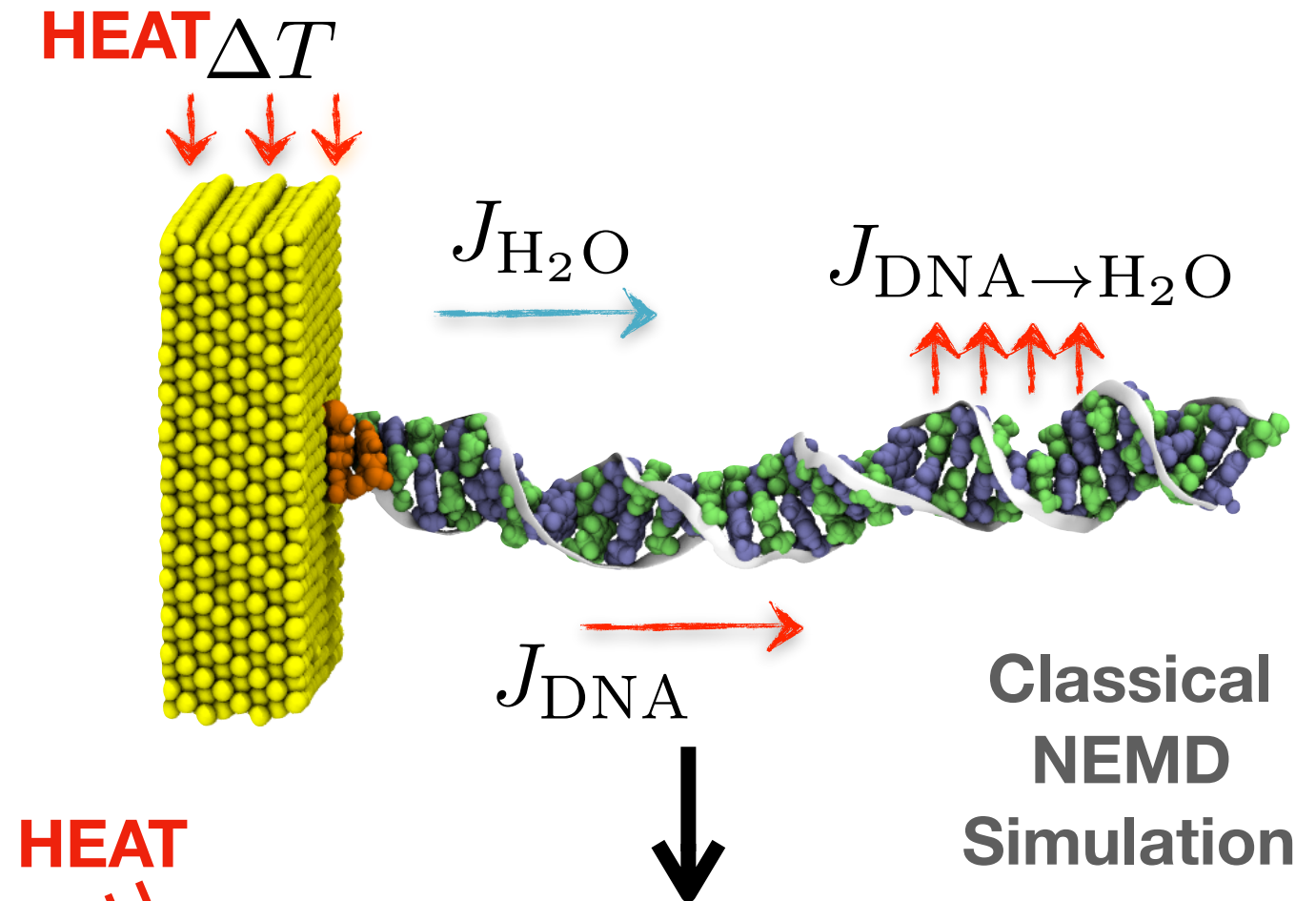


Nucleic acid  
sidechains  
(dynamic hydrogen  
bond topology)



Sugar-phosphate  
backbone  
(fixed topology)

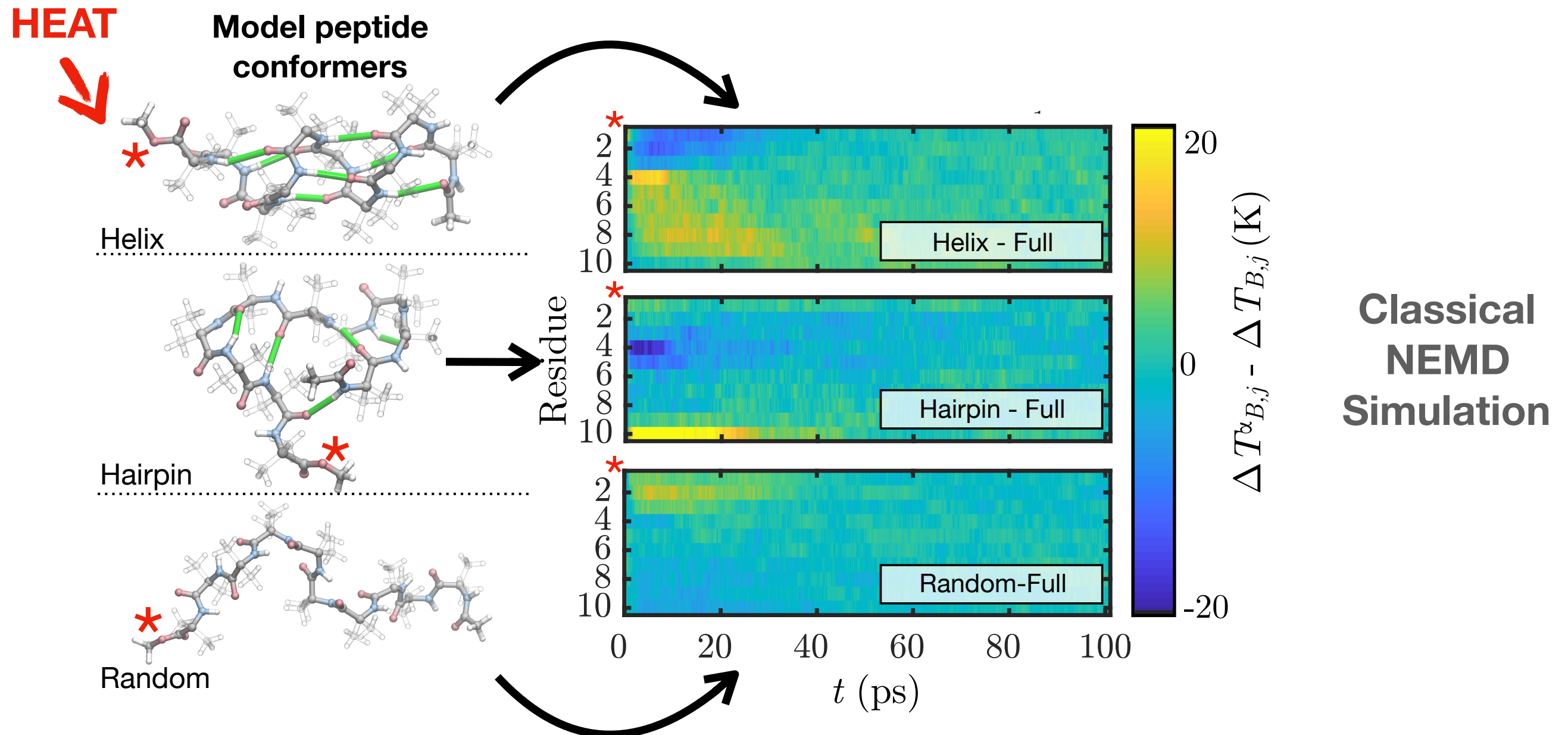
Nonequilibrium molecular simulation reveals dynamic pathways for energy propagation.



# Nonequilibrium Transport in Nonlinear Media:

## Collective and Diffusive Thermal Transport in DNA

*New energy landscape methods are needed for nonequilibrium nanoscale simulation.*



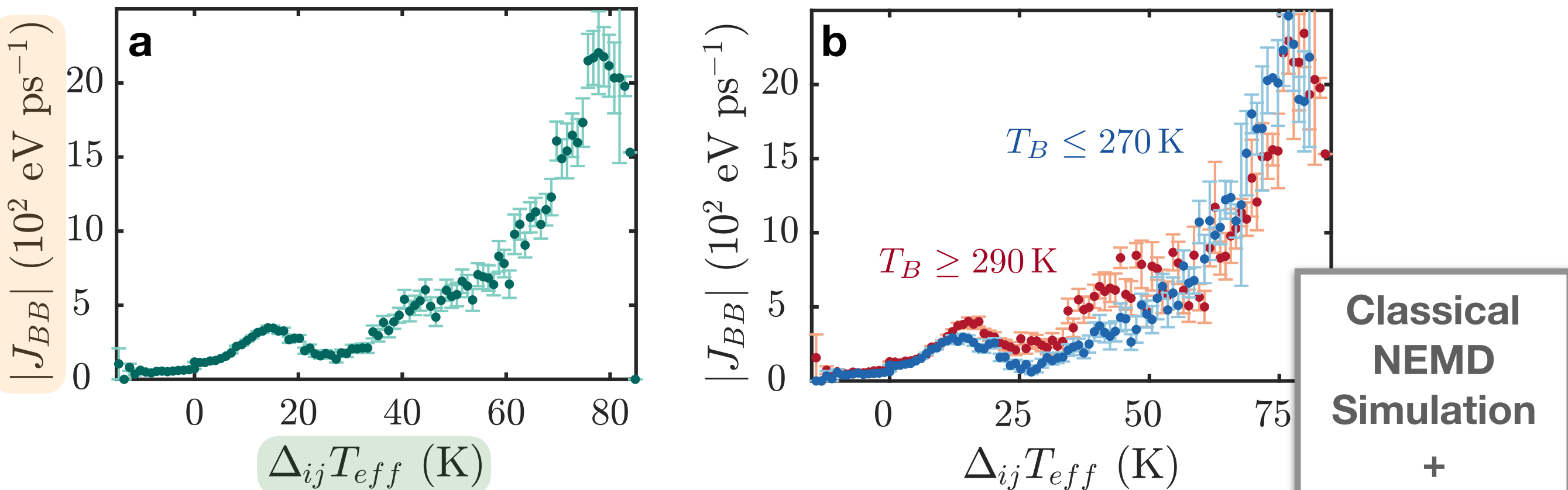
Structural connectivity determines thermal transport profiles for different conformational ensembles.



# Nonequilibrium Transport in Nonlinear Media:

## Collective and Diffusive Thermal Transport in DNA

*Scaling of backbone fluxes in high-temperature and low-temperature regimes probes energy landscape geometry.*



a) Master equation approach can quantify **transient fluxes** versus **local temperature gradient**.

b) Probes energy landscape properties through bath temperature dependence in simulation...  
...or in experiment!

**Classical  
NEMD  
Simulation  
+  
Dynamic  
Master  
Equation  
Analysis**